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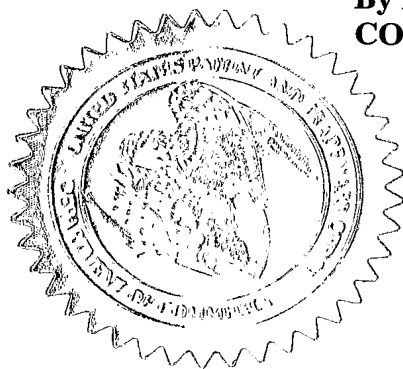
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**PROVISIONAL APPLICATION FOR PATENT COVER SHEET**

This is a request for filing a PROVISIONAL APPLICATION FOR PATENT under 37 CFR 1.53(c).

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Additional inventors are being named on the _____ separately numbered sheets attached hereto					
TITLE OF THE INVENTION (500 characters max)					
Fast Quantum Mechanical Initial State Approximation					
Direct all correspondence to: CORRESPONDENCE ADDRESS					
<input checked="" type="checkbox"/> Customer Number: 28089					
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ENCLOSED APPLICATION PARTS (check all that apply)					
<input checked="" type="checkbox"/> Specification Number of Pages 14		<input type="checkbox"/> CD(s), Number _____			
<input checked="" type="checkbox"/> Drawing(s) Number of Sheets 2		<input checked="" type="checkbox"/> Other (specify) Postcard			
<input checked="" type="checkbox"/> Application Date Sheet. See 37 CFR 1.76 (2 pages)					
METHOD OF PAYMENT OF FILING FEES FOR THIS PROVISIONAL APPLICATION FOR PATENT					
<input checked="" type="checkbox"/> Applicant claims small entity status. See 37 CFR 1.27.		FILING FEE Amount (\$)			
<input type="checkbox"/> A check or money order is enclosed to cover the filing fees.		80.00			
<input checked="" type="checkbox"/> The Director is hereby authorized to charge filing fees or credit any overpayment to Deposit Account Number: 08-0219					
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The invention was made by an agency of the United States Government or under a contract with an agency of the United States Government.					
<input type="checkbox"/> No.		US Air Force, Air Force Material Command, Air Force Research			
<input checked="" type="checkbox"/> Yes, the name of the U.S. Government agency and the Government contract number are:		Laboratory/IFKF, Contract No.: F30602-01-0523			

Respectfully submitted,

[Page 1 of 2]

Date 12/15/2003

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(if appropriate) Docket Number: P-00040-1 (019240.171 US2)

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U.S. Patent and Trademark Office; U.S. DEPARTMENT OF COMMERCE**FEE TRANSMITTAL**  
**for FY 2004**

Effective 10/01/2003. Patent fees are subject to annual revision.

☒ Applicant claims small entity status. See 37 CFR 1.27**TOTAL AMOUNT OF PAYMENT** (\$) 80.00**C mplete if Known**

Application Number	TBA
Filing Date	12/15/2003
First Named Inventor	Anargyros Papageorgiou
Examiner Name	N/A
Art Unit	N/A
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**METHOD OF PAYMENT (check all that apply)**☐ Check ☐ Credit card ☐ Money Order ☐ Other ☐ None☒ Deposit Account:Deposit  
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08-0219

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☒ Charge fee(s) indicated below ☒ Credit any overpayments☒ Charge any additional fee(s) or any underpayment of fee(s)☐ Charge fee(s) indicated below, except for the filing fee to the above-identified deposit account.**FEE CALCULATION****1. BASIC FILING FEE**

Large Entity Fee Code (\$)	Small Entity Fee Code (\$)	Fee Description	Fee Paid
1001 770	2001 385	Utility filing fee	
1002 340	2002 170	Design filing fee	
1003 530	2003 265	Plant filing fee	
1004 770	2004 385	Reissue filing fee	
1005 160	2005 80	Provisional filing fee	80.00
<b>SUBTOTAL (1)</b>			<b>(\$)</b> 80.00

**2. EXTRA CLAIM FEES FOR UTILITY AND REISSUE**

Total Claims	Extra Claims	Fee from below	Fee Paid
Independent	-20** =	X	
Multiple Dependent	-3** =	X	
		0	0

Large Entity Fee Code (\$)	Small Entity Fee Code (\$)	Fee Description	Fee Paid
1202 18	2202 9	Claims in excess of 20	
1201 86	2201 43	Independent claims in excess of 3	
1203 290	2203 145	Multiple dependent claim, if not paid	
1204 86	2204 43	** Reissue independent claims over original patent	
1205 18	2205 9	** Reissue claims in excess of 20 and over original patent	
<b>SUBTOTAL (2)</b>			<b>(\$)</b> 0.00

\*\*or number previously paid, if greater; For Reissues, see above

**FEE CALCULATION (continued)****3. ADDITIONAL FEES**

Large Entity Fee Code (\$)	Small Entity Fee Code (\$)	Fee Description	Fee Paid
1051 130	2051 65	Surcharge - late filing fee or oath	
1052 50	2052 25	Surcharge - late provisional filing fee or cover sheet	
1053 130	1053 130	Non-English specification	
1812 2,520	1812 2,520	For filing a request for <i>ex parte</i> reexamination	
1804 920*	1804 920*	Requesting publication of SIR prior to Examiner action	
1805 1,840*	1805 1,840*	Requesting publication of SIR after Examiner action	
1251 110	2251 55	Extension for reply within first month	
1252 420	2252 210	Extension for reply within second month	
1253 950	2253 475	Extension for reply within third month	
1254 1,480	2254 740	Extension for reply within fourth month	
1255 2,010	2255 1,005	Extension for reply within fifth month	
1401 330	2401 165	Notice of Appeal	
1402 330	2402 165	Filing a brief in support of an appeal	
1403 290	2403 145	Request for oral hearing	
1451 1,510	1451 1,510	Petition to institute a public use proceeding	
1452 110	2452 55	Petition to revive - unavoidable	
1453 1,330	2453 665	Petition to revive - unintentional	
1501 1,330	2501 665	Utility issue fee (or reissue)	
1502 480	2502 240	Design issue fee	
1503 640	2503 320	Plant issue fee	
1460 130	1460 130	Petitions to the Commissioner	
1807 50	1807 50	Processing fee under 37 CFR 1.17(q)	
1806 180	1806 180	Submission of Information Disclosure Stmt	
8021 40	8021 40	Recording each patent assignment per property (times number of properties)	
1809 770	2809 385	Filing a submission after final rejection (37 CFR 1.129(a))	
1810 770	2810 385	For each additional invention to be examined (37 CFR 1.129(b))	
1801 770	2801 385	Request for Continued Examination (RCE)	
1802 900	1802 900	Request for expedited examination of a design application	

Other fee (specify)

\*Reduced by Basic Filing Fee Paid

**SUBTOTAL (3)** (\$) 0.00**SUBMITTED BY**

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**Application Data Sheet**

**Application Information**

Application Type:: Provisional  
Subject Matter:: Utility  
Title:: FAST QUANTUM MECHANICAL INITIAL STATE APPROXIMATION  
  
Attorney Docket Number:: P-00040-1 (019240.171 US2)  
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Licensed US Govt. Agency:: US Air Force, Air Force Material Command, Air Force Research Laboratory/IFKF  
  
Contract or Grant Numbers:: F30602-01-0523  
Secrecy Order in Parent Appl.?:: No

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## FAST QUANTUM MECHANICAL INITIAL STATE APPROXIMATION

### GOVERNMENT INTERESTS

This application discloses an invention made with government support under Contract No. F30602-01-0523 awarded by US Air Force, Air Force Material Command Air Force Research Laboratory/IFKF. The government may have certain rights in the invention.

### FIELD OF THE INVENTION

This invention relates to quantum computing and to methods and systems to efficiently calculate eigenvalues and eigenvectors Hermitian operators and quantum mechanical evolution operators with quantum computers and methods and systems to efficiently calculate an approximate quantum state to be used as an input in a quantum mechanical system.

### BACKGROUND

Intuitively, quantum mechanical problems offer great potential for quantum computers to achieve large speedups over classical machines. An important problem of this kind is the approximation of an eigenvalue of a quantum mechanical operator. In a recent paper published in 1999 in Physical Review Letters (Vol 83, p. 5162) and hereby incorporated by reference, Abrams and Lloyd present a quantum method for doing this. Their method is exponentially faster than the best classical method, but requires a good approximation of the corresponding eigenvector as an input.

There is currently a continuing need for a method and system for efficiently computing a good approximation of the eigenvector as an input to the Abrams and Lloyd quantum method.

There is also a continuing need for a method and system for efficiently computing a good approximation of a quantum state (not limited to eigenvectors) as an input to a quantum mechanical computer or computation. For example, one would like to compute an approximate input to the quantum simulation algorithm. The quantum simulation algorithm is described in the book Quantum Computation and Quantum Information, by M. A. Nielsen and I. L. Chuang, Cambridge University Press, Cambridge UK (2000).

### SUMMARY OF THE INVENTION

The present invention is a system and method for use on a quantum computer to efficiently prepare the initial quantum state required by Abrams and Lloyd's eigenvalue approximation method. The system and method of the present invention is used to prepare a quantum register with an approximation of the eigenvector that is guaranteed to be sufficiently good to be used as input to the Abrams and Lloyd method. The present invention can be used when solving continuous Hermitian eigenproblems, e.g. the Schrödinger equation, on a discrete grid.

Beginning with an eigenvector for a problem discretized on a coarse grid, the system of the present invention efficiently constructs, quantum mechanically, an approximation of the same eigenvector on a finer grid. This eigenvector approximation is suitable as the initial state for the eigenvalue estimation method of Abrams and Lloyd.

Similarly beginning with a vector (i.e., a quantum state) for a continuous problem discretized on a coarse grid, the system of the present invention efficiently constructs, quantum mechanically, a vector (i.e., a state), which is an approximation to the

corresponding vector on a finer grid. Our system efficiently extends a vector of low dimension to one of high dimension, which is then presented as input to some quantum computation method, e.g., the quantum simulation algorithm.

The features and advantages of the present invention will be more readily apparent and understood from the following detailed description of the invention, which should be understood in conjunction with the accompanying drawings appended to the end of the detailed description.

### **BRIEF DESCRIPTION OF THE DRAWINGS**

Figure 1 is a chart illustrating the steps performed on the various quantum registers according to an embodiment of the present invention.

Figure 2 is a chart illustrating the steps performed on the various quantum registers according to another embodiment of the invention.

### **DETAILED DESCRIPTION**

For purposes of illustration only, and not to limit the scope of the present invention, the invention will be explained with reference to the embodiments of the invention indicated in the drawings. One skilled in the art would understand that the present invention is not limited to the specific examples disclosed and can be more generally applied to other initial state preparation methods and systems than those disclosed.

The key component in the Abrams and Lloyd method is quantum phase estimation, which is a method for approximating an eigenvalue of a unitary matrix. Quantum phase estimation is also described in the above referenced book of Nielsen and Chuang. We give a brief outline of this method below.



Let  $Q$  denote a  $2^m \times 2^m$  unitary matrix. We want to approximate a specific eigenvalue of  $Q$ . Phase estimation does this using the corresponding eigenvector as input. The Abrams and Lloyd method deals with the case when this eigenvector is not known exactly. Referring to Figure 1, consider a quantum computer consisting of three registers 140, 150, and 160 with a total of  $b + m + w$  qubits. The first  $b$  qubits in register 150 are all initially in the state  $|0\rangle$ . The second register 140 with  $m$  qubits is initialized to some state  $|\psi\rangle$ , which must approximate the eigenvector in question sufficiently well, as will be seen. The last  $w$  qubits in register 160 are work qubits for temporary storage. The  $w$  qubits are not important in our discussion here, and we generally omit discussion of them below.

Since  $Q$  is unitary and therefore normal, the state  $|\psi\rangle$  can be expanded with respect to eigenvectors of  $Q$ . Omitting discussion of the work qubits in register 160, the initial state of the algorithm is

$$|0\rangle|\psi\rangle = |0\rangle \sum_u d_u |u\rangle, \quad (1)$$

where  $|u\rangle$  are the eigenvectors of  $Q$ . Placing the first register 150 in an equal superposition, using  $b$  Hadamard gates in step 170, transforms this state into

$$\frac{1}{\sqrt{2^b}} \sum_{j=0}^{2^b-1} |j\rangle \sum_u d_u |u\rangle. \quad (2)$$

Next, powers of  $Q$  are applied in step 170 to create the state

$$\frac{1}{\sqrt{2^b}} \sum_{j=0}^{2^b-1} |j\rangle Q^j \sum_u d_u |u\rangle. \quad (3)$$

Since  $Q$  is unitary, its eigenvalues can be written as  $e^{2\pi i \varphi_u}$ , where  $\varphi_u \in \mathbb{R}$ . We can assume that  $\varphi_u \in [0,1)$  and consider the approximation of one of these phases instead of the approximation of one of the eigenvalues. Equation (3) is equal to

$$\frac{1}{\sqrt{2^b}} \sum_u \sum_{j=0}^{2^b-1} d_u e^{2\pi i j \varphi_u} |j\rangle |u\rangle. \quad (4)$$

It is easily seen that the inverse Fourier transform performed in step 170 on the first register 150 creates the state

$$\sum_u d_u \left( \sum_{j=0}^{2^b-1} g(\varphi_u, j) |j\rangle \right) |u\rangle, \quad (5)$$

where

$$g(\varphi_u, j) = \begin{cases} \frac{\sin(\pi(2^b \varphi_u - j)) e^{\pi i (\varphi_u - j 2^{-b})(2^b - 1)}}{2^b \sin(\pi(\varphi_u - j 2^{-b}))}, & 2^b \varphi_u \neq j \\ 1, & 2^b \varphi_u = j. \end{cases} \quad (6)$$

In step 180, a measurement of the first register 150 produces outcome  $j$  190 with probability

$$p_j = \sum_u |d_u|^2 |g(\varphi_u, j)|^2, \quad (7)$$

and the second register 140 will collapse to the state

$$\sum_u \frac{d_u g(\varphi_u, j)}{\sqrt{p_j}} |u\rangle. \quad (8)$$

represented by the register 200; register 210 contains the work qubits after the measurement 180 as known to one skilled in the art.

We remark that for special case when the eigenvalues  $\varphi_u$  can be represented exactly with  $b$ -bits (i.e.,  $2^b \varphi_u$  is an integer), equation (5) simplifies to

$$\sum_u d_u |\varphi_u\rangle |u\rangle. \quad (9)$$

When the eigenvalues are of this form and are distinct, a measurement in step 180 of the first register 150 will cause the second register 140 to collapse exactly onto the corresponding eigenvector in register 200.

Recall that the system and method of the present invention are to achieve an approximation of the phase that corresponds to an eigenvector  $|u\rangle$  using a quantum computer, that the state  $|\psi\rangle$  is an approximation of this eigenvector, and that the eigenvalue is obtained from the value of the outcome  $j$  190 by  $e^{2\pi i j/2^b}$  is of the form and approximates  $e^{2\pi i \varphi_u}$ . For instance, one is often interested in the eigenvalue corresponding to the ground state or in low order eigenvalues. We define  $\Delta(\varphi_0, \varphi_1) = \min_{x \in \mathbb{Z}} \{ |x + \varphi_1 - \varphi_0| \}$ ,  $\varphi_0, \varphi_1 \in \mathbb{R}$  (i.e., the fractional part of the distance between  $\varphi_0$  and  $\varphi_1$ ). Then a measurement of the first register produces an outcome from the set  $G = \{j : \Delta(j/2^b, \varphi_u) \leq k/2^b, k > 1\}$  with probability

$$\begin{aligned} \Pr(G) &= \sum_{j \in G} \sum_u |d_u g(\varphi_u, j)|^2 \\ &\geq \sum_{j \in G} |d_{u'} g(\varphi_{u'}, j)|^2 \\ &\geq |d_{u'}|^2 - \frac{|d_{u'}|^2}{2(k-1)}, \end{aligned} \quad (10)$$

and when  $k = 1$  the probability to obtain  $j$  such that  $\Delta(j/2^b, \varphi_u) \leq 2^{-b}$  is bounded from below by  $\frac{8}{\pi^2} |d_u|^2$ .  $|\psi\rangle$  must be chosen in a way that this probability is large or preferably greater than  $1/2$ , which implies that  $|d_u|$  has to be sufficiently large. For one embodiment of the present invention to obtain an approximation of  $\varphi_u$  with accuracy  $2^{-n}$  and probability at least  $|d_u|^2 (1 - \epsilon)$ , equation (10) shows that the number of qubits  $b$  in the first register **150** must be

$$b = n + \left\lceil \log \left( 1 + \frac{1}{2\epsilon} \right) \right\rceil. \quad (11)$$

Quantum phase estimation can be used as an efficient subroutine to find eigenvalues. Consider a Hermitian operator  $H$ . The operator  $G(t) = e^{-iHt}$  is unitary and has the same eigenvectors as  $H$ . We assume that  $G$  can be implemented efficiently and, therefore, can be used as the unitary operator in the phase estimation algorithm. For example, when  $H$  is local, i.e., it can be written in the form  $\sum H_j$ , where each  $H_j$  acts only on a small number of qubits, then  $G$  can be implemented efficiently. However, locality is not a necessary condition for efficient implementation. Indeed,  $G$  can be efficiently implemented for a many-particle quantum mechanical system with a non-local  $H$ . One skilled in the art will understand that it is possible to implement  $G$  for a wide class of non-local Hamiltonians.

The Hermitian eigenproblem described above is solved on a discrete grid. One embodiment of the present invention addresses the case in which the grid is extremely fine. Clearly, a fine grid requires a large vector for the representation of the initial state of the algorithm. In general, it may not be possible to efficiently prepare an arbitrary

quantum state in a space with a large number of qubits. However, the present invention includes a method for the efficient preparation of an initial state.

In one embodiment of the invention, the operator possesses an eigenvector for a coarse grid discretization of the problem, which was most likely obtained classically since the size of the problem is small, although one skilled in the art will understand an eigenvector obtained by any coarse method can be employed without diverging from the scope of the invention. Using this eigenvector, we efficiently construct an approximation to the corresponding eigenvector for a fine grid discretization of the problem. We use this approximation as the initial state of the eigenvalue approximation algorithm. We describe our method for a one-dimensional continuous problem on the interval  $[0,1]$ .

Let  $H$  be a positive Hermitian operator, defined on a Hilbert space of smooth functions on  $[0,1]$ . Let  $v_k(\cdot)$ ,  $k = 1, 2, \dots$ , denote the eigenfunctions of  $H$ , ordered according to the magnitude of the corresponding eigenvalues; and without loss of generality we assume that

$$\int_0^1 |v_k(x)|^2 dx = 1. \quad (12)$$

Suppose that  $H_N$  is a discretization of  $H$  with grid size  $h_N = 1/(1 + N)$ . Let

$|U_k^{(N)}\rangle$ ,  $k = 0, 1, \dots, N-1$ , denote the normalized eigenvectors of  $H_N$ , ordered according to the magnitude of the corresponding eigenvalues. The expansion of the  $k$ -th eigenvector in the computational basis can be written as

$$|U_k^{(N)}\rangle = \sum_{j=0}^{N-1} u_{k,j}^{(N)} |j\rangle. \quad (13)$$

Let  $|V_k^{(N)}\rangle = \sum_{j=0}^{N-1} v_k((j+1)h_N) |j\rangle$  be the sampled version of  $v_k(\cdot)$  at the discretization points. Consider problems such that the eigenvector of interest satisfies

$$\|v_k'\|_{\infty} = \sup_{0 \leq x \leq 1} |v_k'(x)| = O(1) \text{ and}$$

$$\left\| |U_k^{(N)}\rangle - \frac{|V_k^{(N)}\rangle}{\|V_k^{(N)}\rangle\|} \right\| = O(h_N^q), \quad (14)$$

where  $q > 0$  is the order of convergence and  $\|X\|^2 = \sum_{j=0}^{N-1} |x_j|^2$  for

$$|X\rangle = \sum_{j=0}^{N-1} x_j |j\rangle. \text{ For example, these conditions are satisfied when, for example,}$$

we are dealing with second order elliptic operators.

Now, assume that the eigenvector  $|U_k^{(N_0)}\rangle$  of  $H_{N_0}$  has been obtained classically.

This vector is placed in a  $\log N_0$  qubit register 110 (see Figure 1). For  $N = 2^s N_0$ , we

construct an approximation  $|\tilde{U}_k^{(N)}\rangle$  of  $|U_k^{(N)}\rangle$  by appending  $s$  qubits in register 120, each

qubit in the state  $|0\rangle$ , to  $|U_k^{(N_0)}\rangle$  and then performing in step 130 a Hadamard

transformation on each one of these  $s$  qubits in register 120, i.e.

$$\begin{aligned} |\tilde{U}_k^{(N)}\rangle &= |U_k^{(N_0)}\rangle \left( \frac{|0\rangle + |1\rangle}{\sqrt{2}} \right)^{\otimes s} \\ &= \frac{1}{\sqrt{2^s}} \sum_{j=0}^{N-1} u_{k,f(j)}^{(N_0)} |j\rangle, \end{aligned} \quad (15)$$

where  $f(j) = \lfloor j/2^s \rfloor$ . The effect of  $f$  is to replicate the coordinates of  $|U_k^{(N_0)}\rangle$   $2^s$  times.

According to the present invention,  $|\tilde{U}_k^{(N)}\rangle$  is used as input to the eigenvalue and

eigenvector approximation method. When the result of the method is measured  $|\tilde{U}_k^{(N)}\rangle$

will collapse onto a superposition of eigenvectors according to equation (8). The magnitude of the coefficient of  $|U_k^{(N)}\rangle$  in this superposition can be made arbitrarily close to one by appropriately choosing  $N_0$ .

Consider two different expansions of  $|\tilde{U}_k^{(N)}\rangle$ :

$$|\tilde{U}_k^{(N)}\rangle = \sum_{j=0}^{N-1} \tilde{u}_{k,j}^{(N)} |j\rangle \quad (16)$$

$$|\tilde{U}_k^{(N)}\rangle = \sum_{l=0}^{N-1} d_{k,l}^{(N)} |U_l^{(N)}\rangle. \quad (17)$$

The first expansion is in the computational basis and the second is with respect to the eigenvectors  $H_N$ . We call  $|d_{k,k}^{(N)}|^2$  the probability of success. Equation (17) can be rewritten as

$$|\tilde{U}_k^{(N)}\rangle - |U_k^{(N)}\rangle = (d_{k,k}^{(N)} - 1)|U_k^{(N)}\rangle + \sum_{l \neq k} d_{k,l}^{(N)} |U_l^{(N)}\rangle. \quad (18)$$

Taking norms on both sides and using (13) and (16) gives the inequality

$$\begin{aligned} \left\| |U_k^{(N)}\rangle - |\tilde{U}_k^{(N)}\rangle \right\|^2 &= \sum_{j=0}^{N-1} |u_{k,j}^{(N)} - \tilde{u}_{k,j}^{(N)}|^2 \\ &= |d_{k,k}^{(N)} - 1|^2 + \sum_{l \neq k} |d_{k,l}^{(N)}|^2 \\ &\geq \sum_{l \neq k} |d_{k,l}^{(N)}|^2 \\ &= 1 - |d_{k,k}^{(N)}|^2. \end{aligned} \quad (19)$$

We will now bound (19) from above, and thus the probability of failure. The definition of  $|\tilde{U}_k^{(N)}\rangle$  implies

$$\left\| |U_k^{(N)}\rangle - |\tilde{U}_k^{(N)}\rangle \right\|^2 = \sum_{j=0}^{N-1} \left| \frac{v_k((j+1)h_N)}{\|V_k^{(N)}\|} - \frac{v_k((f(j)+1)h_{N_0})}{\sqrt{2^s}\|V_k^{(N_0)}\|} + \Delta_{k,j}^{(N)} - \frac{\Delta_{k,f(j)}^{(N_0)}}{\sqrt{2^s}} \right|^2, \quad (20)$$

where  $\sum_{j=0}^{N-1} |\Delta_{k,j}^{(N)}|^2 = O(h_N^{2q})$  and  $\sum_{j=0}^{N-1} |\Delta_{k,f(j)}^{(N_0)}|^2 = 2^s O(h_{N_0}^{2q})$  by (14). Applying the triangle inequality, we get

$$\left\| |U_k^{(N)}\rangle - |\tilde{U}_k^{(N)}\rangle \right\| \leq \left( \sum_{j=0}^{N-1} \left| \frac{v_k((j+1)h_N)}{\|V_k^{(N)}\|} - \frac{v_k((f(j)+1)h_{N_0})}{\sqrt{2^s}\|V_k^{(N_0)}\|} \right|^2 \right)^{1/2} + O(h_{N_0}^q). \quad (21)$$

The definition of  $|V_k^{(N)}\rangle$  and the fact that  $\|v_k\|_\infty = O(1)$  imply that

$\|V_k^{(N)}\| = \sqrt{N}(1 + O(h_N))$ . Hence, the sum above is equal to

$$\frac{1}{N} \sum_{j=0}^{N-1} |v_k((j+1)h_N)(1 + O(h_N)) - v_k((f(j)+1)h_{N_0})(1 + O(h_{N_0}))|^2. \quad (22)$$

Since  $v_k(\cdot)$  is continuous with a bounded first derivative, we have that

$$v_k(x_{2,j}) = v_k(x_{1,j}) + O(|x_{2,j} - x_{1,j}|), \quad (23)$$

where  $x_{1,j} = (j+1)h_N$  and  $x_{2,j} = (f(j)+1)h_{N_0}$ ,  $j = 0, \dots, N-1$ . Clearly

$|x_{2,j} - x_{1,j}| = O(h_{N_0})$ . Using (22), (23) and the triangle inequality, we obtain from (21)

that

$$\left\| |U_k^{(N)}\rangle - |\tilde{U}_k^{(N)}\rangle \right\| \leq O(h_{N_0}) \frac{\|V_k^{(N)}\|}{\sqrt{N}} + O(h_{N_0}) + O(h_{N_0}^q) = O(h_{N_0}^{\min\{1,q\}}). \quad (24)$$

Hence, the probability of failure is bounded from above by  $O(N_0^{-\min\{2,2q\}})$ . It depends only on the order of convergence to the continuous problem and the number of points in the classically solved small problem. We can select an  $N_0$  such that the



probability of failure is less than  $\frac{1}{2}$ , no matter how much larger  $N$  is. By choosing a large  $N$ , we can make the discretization error arbitrarily small. Equation (24) implies that the probability of obtaining the eigenvalue  $e^{2\pi i \phi_k}$  with accuracy  $2^{-b}$  is at least

$$\frac{8}{\pi^2} (1 - O(N_0^{-\min\{2, 2q\}})).$$

We remark that any classical numerical algorithm that computes an eigenvalue, satisfying a specific (nontrivial) property, of a  $N \times N$  unitary matrix takes time  $\Omega(N)$ . For example, one may want to find the eigenvalue that corresponds to the ground state. This is true even if a matrix is sparse and regardless of whether the algorithm is deterministic or randomized. It is merely a consequence of the fact that the algorithm needs to consider all the (nonzero) elements of the matrix, and there are at least  $\Omega(N)$  such elements. Alternatively, in the restricted case when the matrix is diagonal finding one of its elements is a problem at least as hard as searching an unordered list. The lower bound for searching yields the lower bound in our case.

In conclusion, our method provides a highly efficient preparation of initial states for eigenvalue approximation, requiring only a small number of Hadamard gates. Thus the method of Abrams and Lloyd, using the initial state prepared by the system and method of the present invention, computes the eigenvalue exponentially faster than any classical algorithm. The method of the invention can be generalized to higher dimensional continuous problems.

In another embodiment of the invention, if we possess a vector that corresponds to a coarse discretization of a continuous problem then, under suitable conditions, we can efficiently extend it to a vector that approximates the corresponding vector (i.e., a state) of a fine discretization. Referring to Figure 2, we first place the original or given vector in

register **310**. Assuming that the vector has dimension  $N_0$  this register has  $\log N_0$  qubits. For a  $N = 2^s N_0$ , we append to register **310**  $s$  qubits, in the state  $|0\rangle$ , in register **320**. Then in step **330** we apply the Hadamard transform to the appended qubits. See Equation (15) and the explanation of the effect of the replicating function  $f$ . In register **340** we have the combination of the two registers **310**, **320**, register **340** containing the approximation corresponding to a vector (i.e., state) of dimension  $N = 2^s N_0$ . This requires  $\log N = \log N_0 + s$  qubits for its quantum mechanical representation. Step **350** represents a quantum mechanical system using the approximation obtained in register **340**. Step **360** represents the final state of the system **350**.

Having described the embodiments of the invention, it should be apparent that various combinations of embodiments may be made or modifications added thereto as is known to those skilled in the art without departing from the spirit and scope of the invention.

## FAST QUANTUM MECHANICAL INITIAL STATE APPROXIMATION

### ABSTRACT

A system and method efficiently prepare the initial state of a quantum computer required by the eigenvalue approximation method of Abrams and Lloyd. The system and method can be applied when solving continuous Hermitian eigenproblems, e.g. the Schrödinger equation, on a discrete grid, and allows for efficient calculation of their eigenvalues with quantum computers. A system and method efficiently prepare an approximate initial state (not limited to eigenvectors) of a quantum computer required by a quantum algorithm as input.

Figure 1

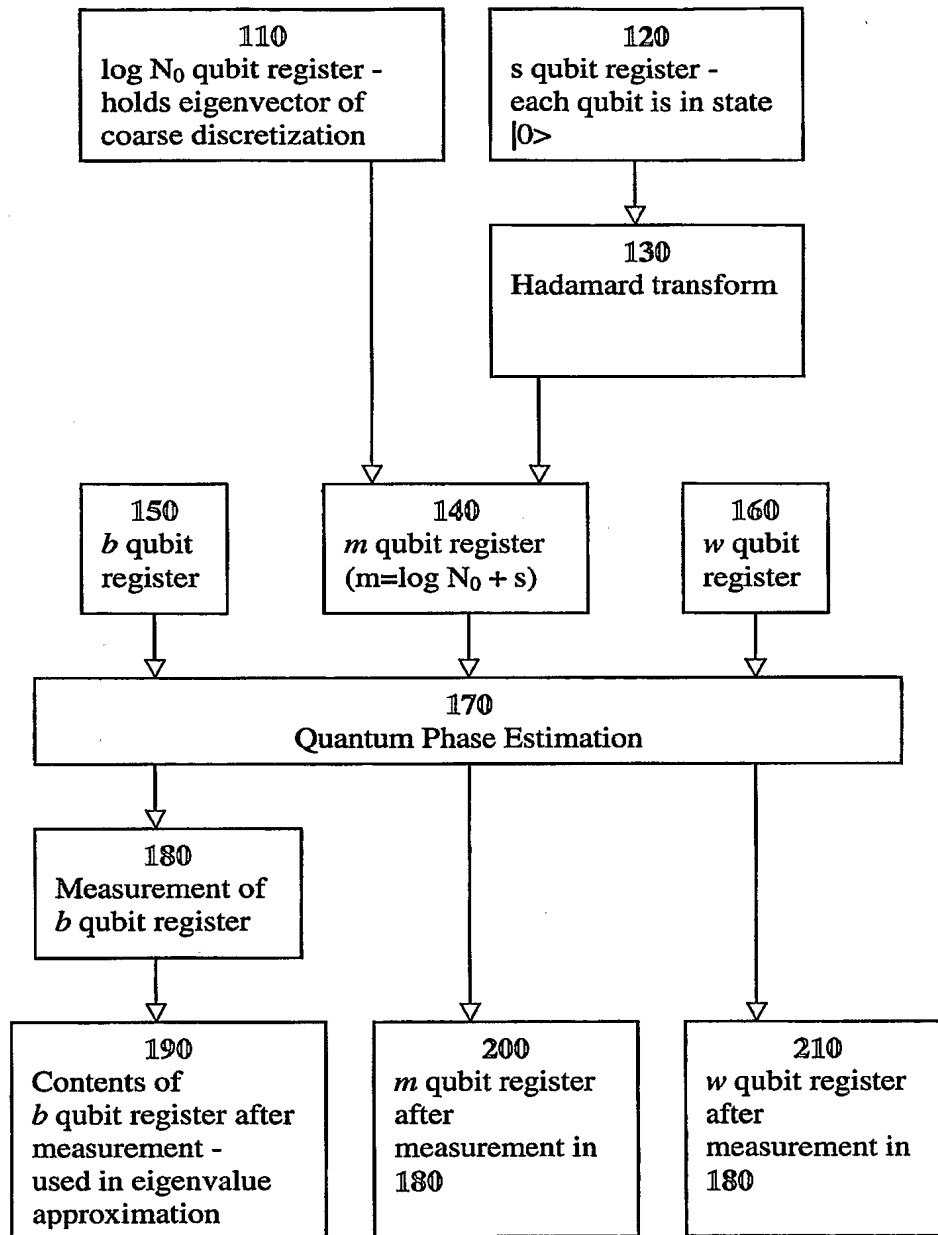
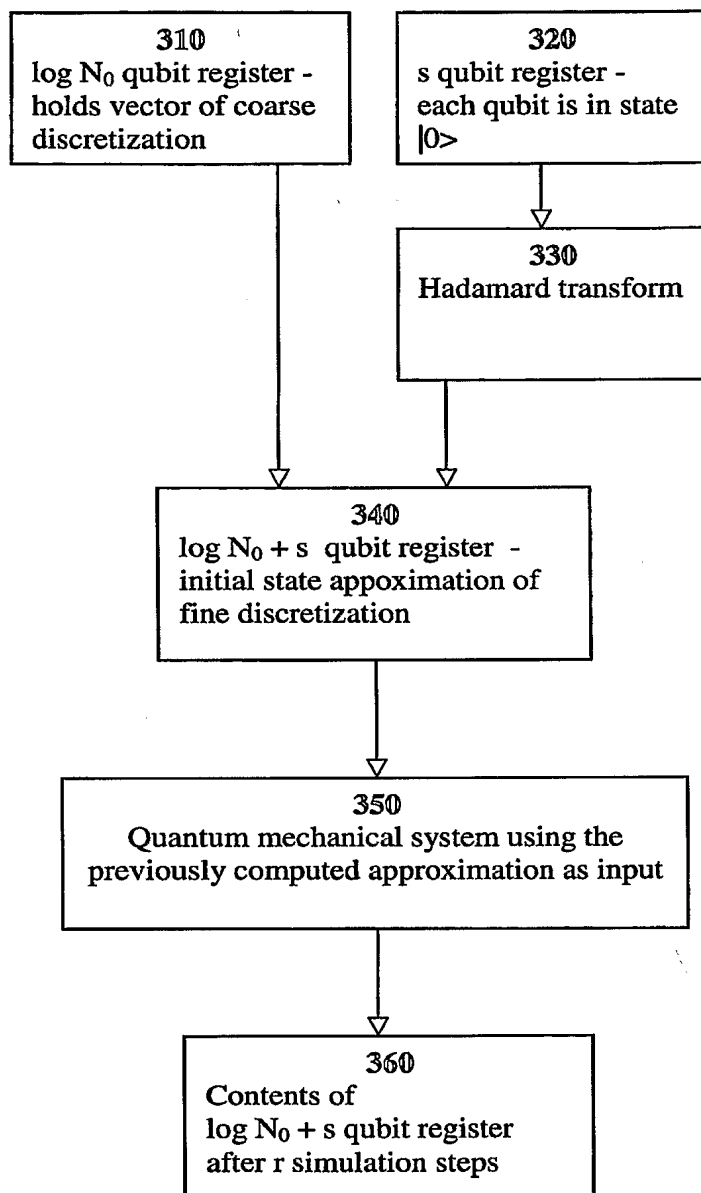


Figure 2



PATENT APPLICATION SERIAL NO. \_\_\_\_\_

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